Organizing Chemical Information to Support Lab Safety

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Abstract:

The Internet provides easy access to a wide variety of information sources relevant to answering chemical safety questions in the laboratory. However, this information is found in a wide variety of formats with varying audiences and intents. This often means that the quality of the information is difficult to evaluate, organize and use to support risk assessment of laboratory work with hazardous chemicals. The ACS Division of Chemical Health and Safety and Division of Chemical Information are partnering to address this concern by developing a chemical safety ontology, or structured vocabulary of terms associated with chemical hazards and risk assessment and management. The goal of this ontology will be to enable the organization of chemical safety information in a sustainable, scalable, and transferable way. This paper will describe the conceptual basis of this work, including the key stakeholders involved, the information channels they use, and their roles in conducting and overseeing the chemical risk assessments in the laboratory.

Introduction

In 1987, OSHA promulgated the Hazard Communication Standard (HCS), which established the requirement for chemical suppliers to provide Material Safety Data Sheets (MSDSs) to people who bought those chemicals. This standard established the “Right to Know” about chemical hazards in workplaces in the United States. In 2013, OSHA announced the first major revision of this standard by incorporating the UN’s Globally Harmonized System (GHS) into the HCS. This change was intended to incorporate the “*Right to Understand*” into the “*Right to Know*”.

The GHS represents a well-defined, user-oriented system of describing chemical hazards, as opposed to traditional MSDS’s, which were generally written “by lawyers, for lawyers”. This legal orientation of MSDS authors often resulted in vague, and often impractical, guidance for the safe use of chemicals. The GHS was developed over a 15 year period by chemistry and safety professionals who recognized that safety information requires both a sound technical basis and good communication practices to be effective.

While the GHS represented a major step forward for the Right to Understand chemical hazards in many settings, it is necessarily built around individual, clearly identified chemicals, used in well-defined ways. These assumptions do not describe many laboratory uses of chemicals, where the concentrations, quantities and identities of materials being used vary widely and change as the laboratory process proceeds. So, while there is significant health and safety information included in the GHS, *it identifies the hazards of specific chemicals*, rather than providing a *hazard analysis of chemical interactions and other safety issues* (such as mechanical, equipment, biological or radiation hazards), or a *risk assessment* associated with specific laboratory work.

Recognizing this problem, the ACS Division of Chemical Health and Safety and Division of Chemical Information have initiated a joint project to help identify electronic information resources available to support a process-oriented approach to chemical health and safety information and to develop a system for providing convenient access to this information for both chemists and the health and safety professionals who support their work. This paper provides a conceptual overview of our work to date and our plans for future development of the ideas discussed.

Part 1: A Clash of Information Models

Traditional laboratory chemical processes tend to involve a number of substances used in irregular ways (see Figure 1).

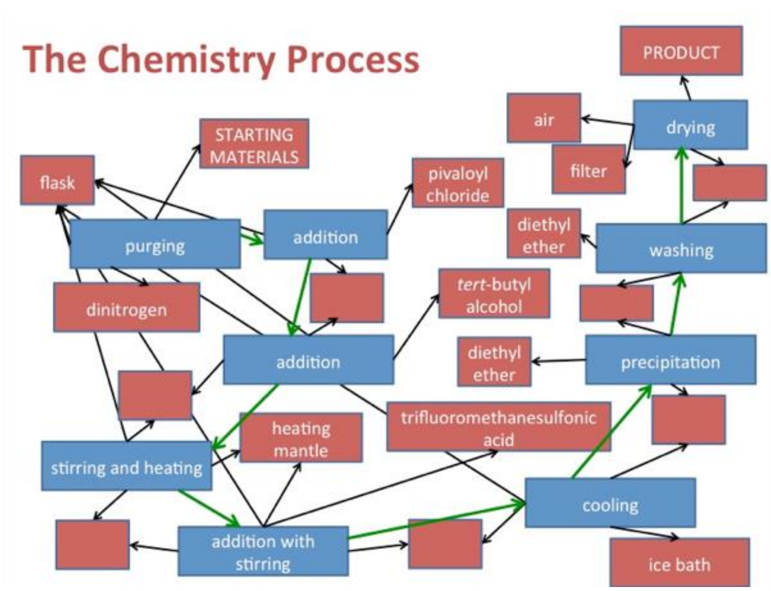

Figure 1: Schematic Overview of a Chemistry Process (Stuart, 2014)

The purpose of these processes is to generate specific chemical changes in these substances that create new substances and/or release or absorb energy, thereby impacting the constituents and environment of the process. These processes may consist of many steps, but they are designed with a particular endpoint in mind. Thus, the laboratory chemical process represents a complicated knowledge domain, the results of which are largely predictable (see Figure 2).

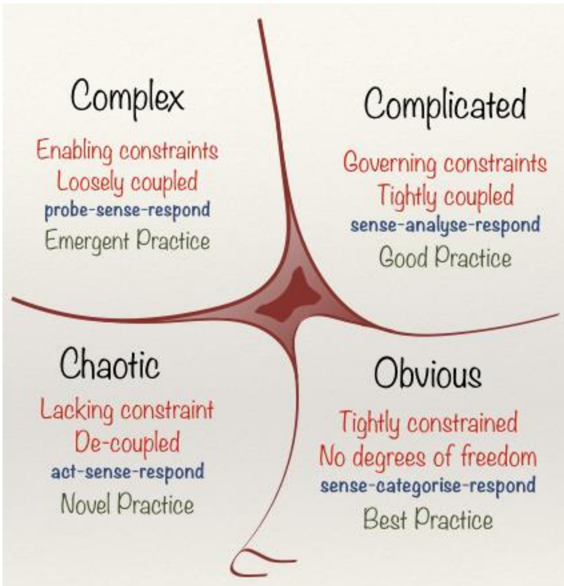

Figure 2: Types of Knowledge Management Domains (Wikipedia, 2014)

While this description of chemical processes is well suited to many activities in the laboratory, it does not describe all work done there. Particularly in the research setting, a chemical process may not have a clear endpoint and unexpected results may arise. Processes with unpredictable results go beyond complicated systems to become complex systems. Happily, many unexpected outcomes of complex systems provide useful results (see the 2014 ACS Reactions Video series for examples). Unfortunately, other unexpected results are less positive (see the US Chemical Safety Board's (CSB) 2011 "Experimenting with Danger" report for three examples).

This clash of information models means that it is necessary to step back and take a broad view of the goal of the risk assessment in order to develop a sustainable information process to support this work. The National Research Council describes this goal as "prudent" chemical practice, as outlined in its *Prudent Practices in the Laboratory* publication. Both practically and legally, such prudence is established by effective documentation of the hazard identification, risk assessment and risk management processes. Such documentation can be used to support the writing of the Standard Operating Procedure and emergency planning guidance required by OSHA as part of the lab standard. With the goal of prudence in mind, the information challenge becomes more tractable.

The laboratory incidents highlighted by the CSB have sparked significant interest in improving the level of laboratory safety education in the college chemistry curriculum (see ACS report on Advancing Graduate Education in the Chemical

Sciences) In particular, industrial employers of chemists are concerned that this curriculum currently provides insufficient education in the process of chemical risk assessment. Unfortunately, conducting and teaching such risk assessments are more of a challenge than they should be. This is for several reasons:

- Common approaches to managing complicated information processes do not transfer smoothly to the complex situations found in many laboratories. The impact of this challenge is indicated by the fact that research laboratories are four times more likely than teaching laboratories to have accidents that require emergency response from public agencies. Research shows that such laboratory emergencies occur three times a week, with widely varying impacts. See my 2012 article in the *Journal of Chemical Health and Safety* for details of these findings.
- Another aspect of the lab safety challenge is represented by the risk assessment and management paradigm itself. Because of the broad range of laboratory hazards, this approach is necessarily broad and relatively simplistic, based on a hierarchy of controls. A more detailed, but still broad, risk assessment process to conduct a chemical risk assessment is described at the UK Health and Safety Executive's COSHH site.
- Also, hazard identification is based on standard hazard data generated outside the laboratory context, so it must be reinterpreted for the laboratory setting, based on the concentration of chemicals, their quantities and environment they are used in.

Information system tools developed over the last decade provide the opportunity to address many of these issues.

Part 2: The Stakeholders

A key element in developing any information process includes careful consideration of the various stakeholders managing and using the process. For simplicity's sake, we identified six broad groups of stakeholders in the laboratory risk assessment process:

1. ***Bench Chemists*** are the people who physically perform lab processes by implementing procedures appropriate to the result desired.
2. ***Laboratory Supervisors*** are people who plan laboratory activities and provide oversight for bench chemists.
3. ***Chemistry Librarians*** provide access to and help with use of chemical information sources for the chemists working in the laboratory
4. ***Chemical Information Scientists*** develop information management systems for chemical data, publications and information.
5. ***Chemical Health and Safety Professionals*** help identify hazards associated with laboratory processes, evaluate risks associated with specific use of the chemicals, and provide advice about appropriate

protective measures to control those hazards, including planning for emergency response in the laboratory.

6. ***Environmental Health and Safety Staff*** merge information developed by Chemical Health and Safety professionals with specific information about laboratory activities within their organization to develop safety programs that serve diverse laboratories in transferrable, scalable and sustainable ways. EHS Staff generally focus on the information needed to provide specific services such as laboratory waste management, safety educational programs and emergency response planning for the universe of laboratories they support.

Most people associated with laboratories play more than one of these roles. For this reason, it's important to note that each of these groups work with different kinds of chemical information and need access to different types of health and safety data and literature. Table 1 outlines this landscape from the various stakeholder perspectives.

Stakeholder	Key Information Channel(s) (see Figure 3)
Bench chemist	Primary sources (raw data, specific Safety Data Sheets, other process specific hazard and biosafety information)
Laboratory Supervisor	Secondary and tertiary sources (Experimental protocols, safety conditions oversight information, skill level of bench chemists they oversee)
Chemistry Librarians	All levels of information sources, including chemistry information tools, such as literature indices; development of search strategies for appropriate safety information
Chemical Information Scientists	Primary and secondary sources (general chemistry as well as machine analysis of specialized information)
Chemical Health and Safety Professionals	Tertiary safety sources (hazard and process information and facility specifications to evaluate risks specific to the process of concern)
Environmental Health and Safety Professionals	Primary safety sources (rosters of chemicals, workers and spaces

	associated with laboratory work in their jurisdiction; emergency plans appropriate to this work)

The diverse nature of this landscape explains why people in multiple roles often find working with safety information a frustrating experience as they try to answer what appears to be a simple question. As Figure 3 illustrates, safety information is associated with different literature sources, which cannot be used interchangeably. For example, the Texas Tech explosion documented in the CSB report demonstrated that the answer to a question about explosion hazards cannot be based only on the name of the chemical and past experience with that chemical, but also the quantity of the material being worked with.

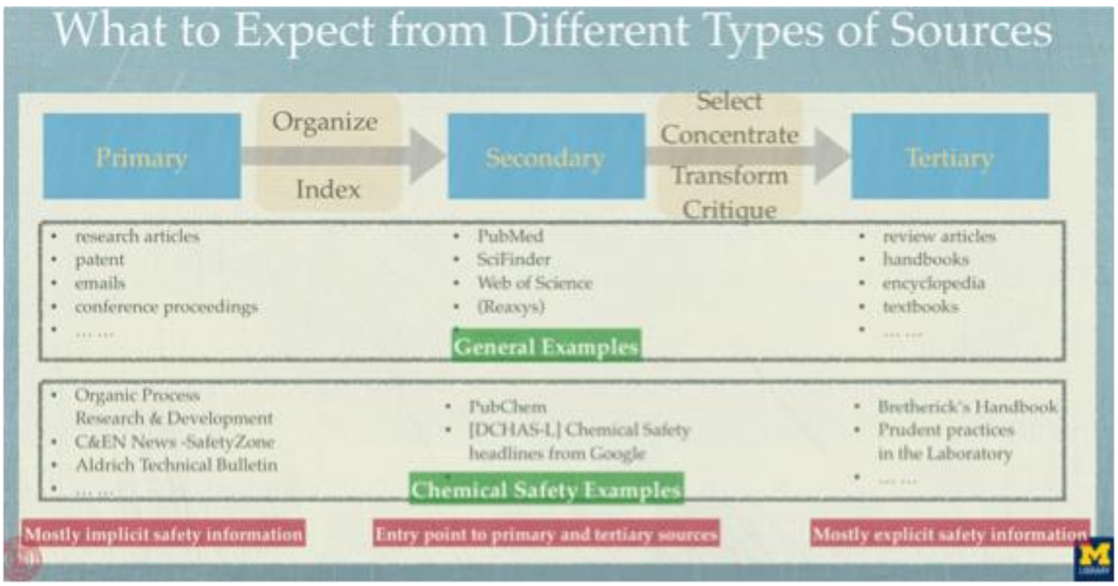

Figure 3: Overview of Chemical Safety Information Sources (Li and McEwen, 2014)

Fortunately, emerging electronic tools, if well planned, will allow the development of more convenient ways to access this information, with some level of intelligent relationships provided to the system. However, because the goal of laboratory safety work is to address unexpected outcomes, there will always be a layer of complexity that requires human judgment beyond the scope of electronic logic, whose strength is found in complicated settings.

Part 3: Information Management Processes

Based on the considerations above, there are two key elements necessary to provide the foundation of a chemical safety information management system. These are *ontologies* and *a curation process.*

In [a 2014 publication,] Colin Batchelor of the Royal Society of Chemistry describes an **ontology** as a "*machine-readable account of what [elements are present] in a given domain and how the things there relate to other things, not necessarily in the most metaphysically general way, but in a way that is consistent with how practicing scientists in that domain understand the relations*". An example of an ontology in action was given in Figure 1.

Curation is a process of expert human review of information according to established guidelines. Such curation often involves manually tagging of specific entities in the ontology to relate them to other items in the system or to information outside the system in ways that machine logic would not identify. This process can become expensive as its scale increases, although new developments in social media present interesting opportunities to address this concern.

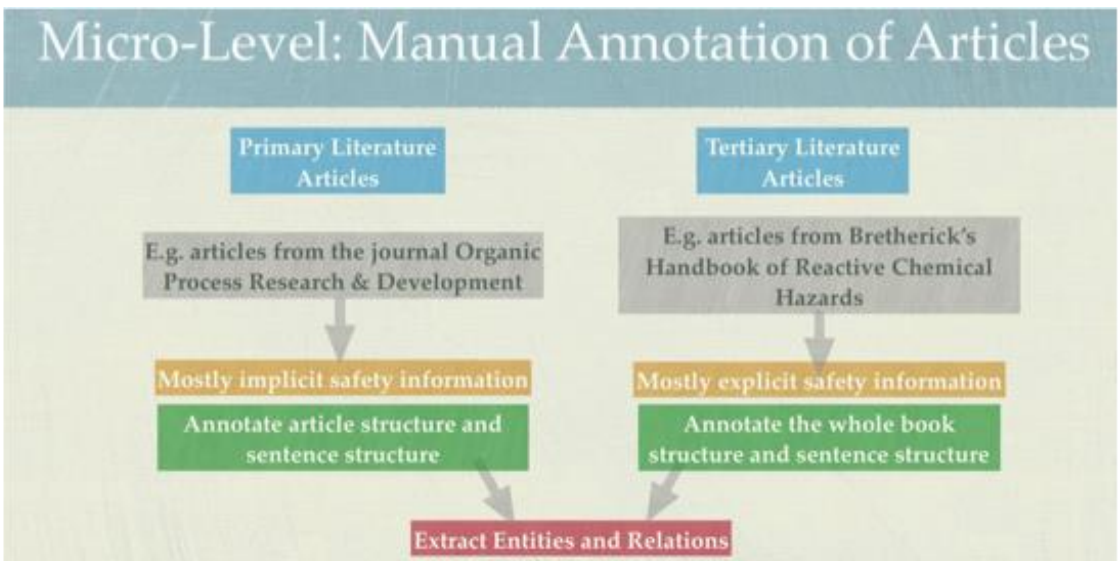

Figure 4: Schematic Overview of Curation Process (Li and McEwen, 2014)

In the safety information context, the ultimate purpose of curation is to produce professional safety advice that supports an operational decision. This judgment is necessary to address the complex (i.e. unpredictable) aspects of the risk assessment process, and, at the professional level, particularly focuses on balancing the costs of managing hazards with the magnitude of the risks they present and identifying specific emergency planning and waste disposal requirements. At a more local level, this information is used to address questions such as matching personal protective equipment requirements to specific laboratory settings.

Developing an information system that incorporates these two elements in a way that matches the expectations of chemists in terms of usability is a challenging task. However, we believe that careful planning of how these elements are implemented is essential to allow such a system to be sustainable as new information technologies become available. Discussions of this project as it proceeds can be found at the iRAMP blog.

Part 4: Two Use Cases

To help make these conceptual considerations more concrete, let's look at two potential use cases for a Chemical Safety Information System. One is the development of Lessons Learned from laboratory accidents; the second is developing a scalable risk assessment tool that can support review of laboratory chemistry for hazard identification and risk management purposes.

Lessons Learned Development

This summer, the National Research Council published a report entitled *Safe Science: Promoting a Culture of Safety in Academic Chemical Research*. One of the recommendations of this report was:

Recommendation 7: Organizations should incorporate non-punitive incident and near-miss reporting as part of their safety cultures. The American Chemical Society, Association of American Universities, Association of Public and Land-grant Universities, and American Council on Education should work together to establish and maintain an anonymous reporting system, building on industry efforts, for centralizing the collection of information about and lessons learned from incidents and near misses in academic laboratories, and linking these data to the scientific literature. Department chairs and university leadership should incorporate the use of this system into their safety planning. Principal investigators should require their students to utilize this system.

A variety of professional organizations and academic institutions have begun development of such systems for laboratories. However, the challenges of developing an organizational system and curation process has made it difficult for such systems to be scaled up in a sustainable way. In order for the NRC recommendation above to be acted upon, the ontology and curation elements described above must be developed with a work flow such as outlined in Figure 5 in mind.

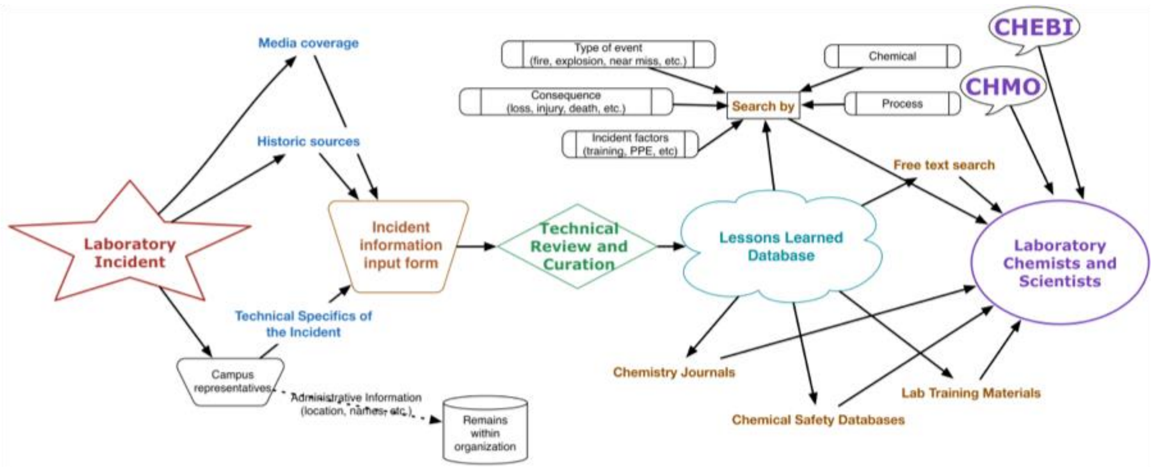

Figure 5: Lessons Learned Collection Workflow (Stuart, 2014)

An example of an ontological approach to the Lessons Learned workflow is provided in Figure 6.

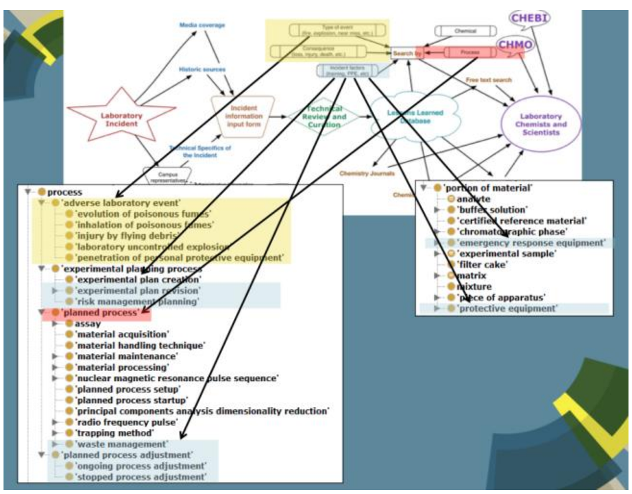

Figure 6: Ontological analysis of Lessons Learned Workflow (Batchelor, 2014)

Scalable Risk Assessment

A second use case for a chemical safety information system is in planning laboratory activities and the safety measures they require. This practice involves several distinct steps for the laboratory supervisor: compilation of data and information to identify the hazards, including properties associated with chemicals and equipment; analysis of the hazards relevant to the specific activities at hand; assessment of the risks within the overall local environment, including training level of the bench chemists; and association of protective measures with various steps in the chemical process.

An interesting aspect of this use case is that the appropriate level of detail for this work to be considered "prudent" will vary based on the risks associated with the procedure being reviewed. The ACS's Committee on Chemical Safety report *"Identifying and Evaluating Hazards in Research Laboratories"* to be released later this year (the link is to the draft version currently available) identifies five such levels of detail (see Figure 7).

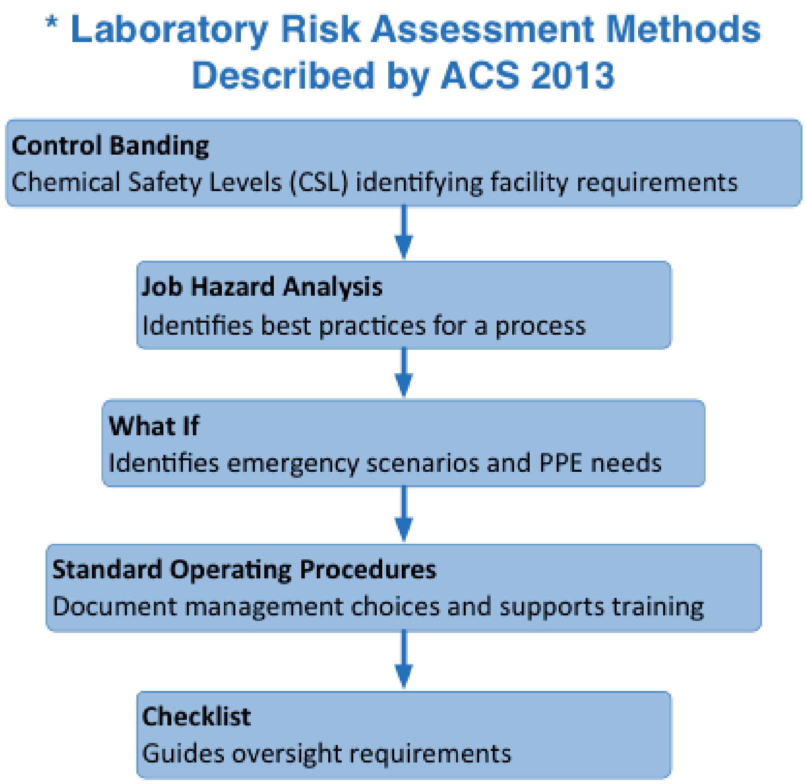

Figure 7: Levels of Detail of Risk Assessment (Stuart, 2014)

These approaches range from relatively simple (for the users) approaches such as control banding to highly detailed approaches such as HAZOP analysis (also known as a "what if" analysis). As an example, the hazard analysis step in the HAZOP workflow is outlined schematically in Table 2.

		Possible Causes and Consequences of:			
Parameter		**More**	**Less**	**None**	**Reverse**
Flow	*causes*	*consequences*			
Temperature	*causes*	*consequences*			
Pressure	*causes*	*consequences*			
Agitation	*causes*	*consequences*			
Venting	*causes*	*consequences*			

Table 2: HAZOP Logic Schematic

Many of the hazardous chemical uses in the laboratory situation do not require the level of detail provided by the HAZOP analysis because the risk they present is limited by the amount of chemical used, the predictability of the chemistry or the amount of supervision provided to the people performing the work. However, even in cases of routine lab-scale chemistry, documenting the risk assessment is a key step in maintaining a safe laboratory. Developing an electronic information system that assists the user in working through this process at the appropriate level of detail will require significant planning and usability testing, but tools appropriate to supporting the development of such a system are becoming more available each year. The first step is to support better linking and searching across the information sources that are available, the first objective of the iRAMP project.

Conclusion

Supporting safe chemical use in the 21st Century laboratory is a complex challenge. A chemical safety information management system can be an important tool in meeting this challenge if it is carefully planned to take advantage of modern information tools in a way that meets chemists' and support needs relative to specific use cases defined as part of the process of developing a prudent laboratory.

Acknowledgements

My thanks to participants at the 2014 Royal Society of Chemistry Chemical Safety Ontology workshop for discussion of these ideas.

Diagram References

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Batchelor, C. "Chemical Safety Ontology" Chemical Safety Ontology Workshop, Cambridge, UK, November 11-13; Royal Society of Chemistry.

Stuart, R. "Supporting Risk Assessment in the Chemistry Lab" Chemical Safety Ontology Workshop, Cambridge, UK, November 11-13; Royal Society of Chemistry.

Links

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